



29 May 1998

Chemical Physics Letters 288 (1998) 891–904

---

---

**CHEMICAL  
PHYSICS  
LETTERS**

---

---

## Author index to volume 288

- Adamowicz, L., see Smith, D.M.A. 288 (1998) 609  
Ågren, H., see Jonsson, D. 288 (1998) 371  
Ahlrichs, R., see Eichkorn, K. 288 (1998) 235  
Allavena, M., see Dziekoński, P. 288 (1998) 538  
Alonso, J.L., see Sanz, M.E. 288 (1998) 760  
An, X., see Li, J. 288 (1998) 175  
Andersson, M., see Granlund, T. 288 (1998) 879  
Andrés, J., see Safont, V.S. 288 (1998) 261  
Antoine, R., A.A. Tamburello-Luca, Ph. Hébert, P.F. Brevet and H.H. Girault, Picosecond dynamics of Eosin B at the air/water interface by time-resolved second harmonic generation: orientational randomization and rotational relaxation 288 (1998) 138  
Aratono, Y., see Kumada, T. 288 (1998) 755  
Artemyev, M.V., see Yumashev, K.V. 288 (1998) 567  
Asakura, K., see Chun, W.-J. 288 (1998) 868  
Ashbrook, S.E., S.P. Brown and S. Wimperis, Multiple-quantum cross-polarization in MAS NMR of quadrupolar nuclei 288 (1998) 509  
Averitt, R.D., see Oldenburg, S.J. 288 (1998) 243  
Aviyente, V., see Selçuki, C. 288 (1998) 669  
Azria, R., see Šiller, L. 288 (1998) 776  
Azuma, J., N. Tamai, A. Shishido and T. Ikeda, Femtosecond dynamics and stimulated emission from the  $S_2$  state of a liquid crystalline trans-azobenzene 288 (1998) 77  
  
Bacis, R., see Campargue, A. 288 (1998) 734  
Bae, S.C., see Lee, K. 288 (1998) 531  
Baer, T., see Mazyar, O.A. 288 (1998) 327  
Balakrishnan, N., A. Dalgarno and G.D. Billing, Multiquantum vibrational transitions in  $O_2(v \geq 25) + O_2(v = 0)$  collisions 288 (1998) 657  
Balasubramanian, K., see Feng, P.Y. 288 (1998) 1  
Barnaba, M., see Carravetta, V. 288 (1998) 37  
Barth, S., H. Bässler, U. Scherf and K. Müllen, Photoconduction in thin films of a ladder-type poly-para-phenylene 288 (1998) 147  
Bässler, H., see Barth, S. 288 (1998) 147  
Batchelor, S.N., Gas-phase EPR of polyatomic radicals 288 (1998) 119  
Bates, M.A., Planar anchoring at the smectic A-isotropic interface. A molecular dynamics simulation study 288 (1998) 209  
Beckert, D., see Geimer, J. 288 (1998) 449  
Ben-Amor, N., S. Evangelisti, D. Maynau and E. Rossi, Benchmark full-CI calculation on  $C_2H_2$ : comparison with (SC)<sup>2</sup>-CI and other truncated-CI approaches 288 (1998) 348

- Berg, L.-E., see Ludwigs, H. 288 (1998) 527
- Berggren, M., see Granlund, T. 288 (1998) 879
- Berndt, T., see Kind, I. 288 (1998) 111
- Bhattacharyya, K., see Pal, S.K. 288 (1998) 793
- Biennier, L., see Campargue, A. 288 (1998) 734
- Billing, G.D., see Balakrishnan, N. 288 (1998) 657
- Björk, G., see Granlund, T. 288 (1998) 879
- Boddenberg, B., see Isfort, O. 288 (1998) 71
- Böge, O., see Kind, I. 288 (1998) 111
- Bolton, K., W.L. Hase, H.B. Schlegel and K. Song, A direct dynamics study of the  $F + C_2H_4 \rightarrow C_2H_3F + H$  product energy distributions 288 (1998) 621
- Bongiovanni, G., M.A. Loi, A. Mura, A. Piaggi, S. Luzzati and M. Catellani, Relaxation processes in thiophene-based random copolymers 288 (1998) 749
- Bouř, P., Calculation of the Raman optical activity via the sum-over-states expansion 288 (1998) 363
- Bower, C., A. Kleinhammes, Y. Wu and O. Zhou, Intercalation and partial exfoliation of single-walled carbon nanotubes by nitric acid 288 (1998) 481
- Braun, T. and H. Rausch, Radioactive endohedral metallofullerenes formed by prompt gamma-generated nuclear recoil implosion 288 (1998) 179
- Brede, O., see Lomoth, R. 288 (1998) 47
- Brevet, P.F., see Antoine, R. 288 (1998) 138
- Brown, S.P., see Ashbrook, S.E. 288 (1998) 509
- Burda, J.V., N. Runeberg and P. Pyykkö, Chemical bonds between noble metals and noble gases. Ab initio study of the neutral diatomics NiXe, PdXe and PtXe 288 (1998) 635
- Burda, J.V., P. Hobza and R. Zahradník,  $(HX)_2$  species ( $X = F$  through At) in the groups of the periodic system:MP2 and CCSD(T) ab initio quantum chemical calculations 288 (1998) 20
- Bussery-Honvault, B., see Campargue, A. 288 (1998) 734
- Caldwell, C.D., see Frigo, S.P. 288 (1998) 98
- Campargue, A., L. Biennier, A. Kachanov, R. Jost, B. Bussery-Honvault, V. Veyret, S. Churassy and R. Bacis, Rotationally resolved absorption spectrum of the  $O_2$  dimer in the visible range 288 (1998) 734
- Campbell, E.E.B., M. Fanti, I.V. Hertel, R. Mitzner and F. Zerbetto, The hyperpolarisability of an endohedral fullerene:  $Li@C_{60}$  288 (1998) 131
- Carravetta, V., G. Polzonetti, G. Iucci, M.V. Russo, G. Paolucci and M. Barnaba, High resolution NEXAFS spectroscopy study of gas-phase phenylacetylene: experiment and theory 288 (1998) 37
- Catellani, M., see Bongiovanni, G. 288 (1998) 749
- Cerezo, C., see Martin, M. 288 (1998) 799
- Cerullo, G., M. Nisoli, S. Stagira, S. De Silvestri, G. Lanzani, W. Graupner, E. List and G. Leising, Ultrafast energy-transfer dynamics in a blend of electroluminescent conjugated polymers 288 (1998) 561
- Chakrabarti, N., see Vandana, K.S. 288 (1998) 545
- Chen, C., see Wang, C. 288 (1998) 473
- Chen, H., see Li, J. 288 (1998) 175
- Choi, J.-H., see Scholefield, M.R. 288 (1998) 487
- Choi, Y.S., see Lim, S.-M. 288 (1998) 828
- Chun, W.-J., K. Asakura and Y. Iwasawa, Anisotropic structure analysis for Mo oxides on  $TiO_2(110)$  single crystal surface by polarization-dependent total-reflection fluorescence EXAFS 288 (1998) 868

- Churassy, S., see Campargue, A. 288 (1998) 734
- Clays, K., G. Olbrechts and A. Persoons, Difference in relaxation time between coherent and incoherent second-harmonic generation 288 (1998) 171
- Cooke, S.A. and A.C. Legon, Rotational spectrum of the trimethylphosphine-hydrogen fluoride complex 288 (1998) 441
- Coriani, S., see Fernández, B. 288 (1998) 677
- Cramer, C.J., see Li, J. 288 (1998) 293
- Cremer, D., see Gräfenstein, J. 288 (1998) 593
- Dag, I., see Lifshitz, E. 288 (1998) 188
- Dai, J., see Wang, C. 288 (1998) 473
- Dalgarno, A., see Balakrishnan, N. 288 (1998) 657
- Danielewicz-Ferchmin, I., A.R. Ferchmin and A. Szlaferek, On the interrelations between charge and mass densities within a double layer 288 (1998) 197
- Datta, A., see Pal, S.K. 288 (1998) 793
- Deng, W.-Q., K.-L. Han, J.-P. Zhan and G.-Z. He, Ab initio and RRKM calculations of *o*-benzyne pyrolysis 288 (1998) 33
- Denifl, G., D. Muigg, A. Stamatovic and T.D. Märk, Dissociative electron attachment to CO and NO: the O<sup>-</sup> production threshold revisited 288 (1998) 105
- Denisov, I.A., see Yumashev, K.V. 288 (1998) 567
- Deniz, A.A., see Lipson, M. 288 (1998) 781
- De Proft, F., see Langenaeker, W. 288 (1998) 628
- De Silvestri, S., see Cerullo, G. 288 (1998) 561
- Díaz-Caro, J., see Torchia, G.A. 288 (1998) 65
- Ding, S. and C.A. McDowell, The equivalence between Floquet formalism and the multi-step approach in computing the evolution operator of a periodical time-dependent Hamiltonian 288 (1998) 230
- Doan, V., V. Tran and B.J. Schwartz, Ultrafast intensity-dependent stimulated emission in conjugated polymers: The mechanism for line-narrowing 288 (1998) 576
- Domingo, L.R., see Safont, V.S. 288 (1998) 261
- Doubinski, A.A., see Poluektov, O.G. 288 (1998) 841
- Dziekoński, P., W.A. Sokalski, E. Kassab and M. Allavena, Electrostatic nature of catalytic effects resulting from Si > Al substitutions in ZMS-5 zeolite 288 (1998) 538
- Eggeling, J., see Mulcahy, C.P.A. 288 (1998) 203
- Eichkorn, K. and R. Ahlrichs, Cadmium selenide semiconductor nanocrystals: a theoretical study 288 (1998) 235
- Elhanine, M., R. Lawruszczuk and B. Soep, Laser spectroscopy of metallic free radicals: the observation of the  $\tilde{C}-\tilde{X}$  vibronically allowed electronic transition for Ca-OCH<sub>3</sub>, Ca-OC<sub>2</sub>H<sub>5</sub> and Ca-CCH 288 (1998) 785
- Elkadi, Y., see Smith, D.M.A. 288 (1998) 609
- Ellinger, Y., see Talbi, D. 288 (1998) 155
- Endo, S., see Sugimoto, T. 288 (1998) 767
- Evangelisti, S., see Ben-Amor, N. 288 (1998) 348
- Fanti, M., see Campbell, E.E.B. 288 (1998) 131
- Fantucci, P., see Jellinek, J. 288 (1998) 705
- Farmanara, P., V. Stert and W. Radloff, Ultrafast internal conversion and fragmentation in electronically excited C<sub>2</sub>H<sub>4</sub> and C<sub>2</sub>H<sub>3</sub>Cl molecules 288 (1998) 518



- Feng, P.Y. and K. Balasubramanian, Electronic states of  $\text{Ga}_3\text{P}$  and  $\text{GaP}_3$  clusters 288 (1998) 1  
Ferchmin, A.R., see Danielewicz-Ferchmin, I. 288 (1998) 197  
Fernández, B., S. Coriani and A. Rizzo, MCSCF polarizability and hyperpolarizabilities of HCl and HBr 288 (1998) 677  
Filatov, M. and S. Shaik, Spin-restricted density functional approach to the open-shell problem 288 (1998) 689  
Finley, J., P.-Å. Malmqvist, B.O. Roos and L. Serrano-Andrés, The multi-state CASPT2 method 288 (1998) 299  
Francisco, J.S., Structure, vibrational spectra and energetics of  $\text{OBrO}^+$  288 (1998) 307  
Friesner, R.A., see Murphy, R.B. 288 (1998) 403  
Frigo, S.P., A. Menzel and C.D. Caldwell, Core to valence transitions in methane 288 (1998) 98  
Fujara, F., see Isfort, O. 288 (1998) 71  
Fujii, R., K. Onaka, M. Kuki, Y. Koyama and Y. Watanabe, The  $2A_g^-$  energies of all-trans-neurosporene and spheroidene as determined by fluorescence spectroscopy 288 (1998) 847  
Fujimura, Y., see Ishida, T. 288 (1998) 433  
Fujiwara, T., see Ishida, T. 288 (1998) 433  
Furuya, K., E. Koto, T. Ueda, K. Maruyama and T. Ogawa, Correlation between  $\text{CH(A)}$  and  $\text{H}^+$  produced by dissociative ionization of ethylene 288 (1998) 816
- Gador, N., see Ludwigs, H. 288 (1998) 527  
Gamperling, M., see Hüttner, W. 288 (1998) 553  
Garcia, E., see Laganà, A. 288 (1998) 616  
Gatehouse, B., Ab initio nuclear shielding parameters and spin-rotation coupling constants of FBO, CIBO and FBS 288 (1998) 698  
Gaumet, J.J., see Lafargue, P.E. 288 (1998) 494  
Gdanitz, R.J., Erratum to "Accurately solving the electronic Schrödinger equation of atoms and molecules using explicitly correlated ( $r_{12}$ -) MR-CI: the ground state potential energy curve of  $\text{N}_2$ ". [Chem. Phys. Lett. 283 (1998) 253] 288 (1998) 590  
Geerlings, P., see Langenaeker, W. 288 (1998) 628  
Geimer, J. and D. Beckert, Study of radical pairs generated by photoreduction of anthraquinone-2,6-disulfonic acid with thymine by Fourier transform electron paramagnetic resonance 288 (1998) 449  
Gerds, T., see Pesce, L. 288 (1998) 383  
Geva, E. and J.L. Skinner, Two-state dynamics of single biomolecules in solution 288 (1998) 225  
Girault, H.H., see Antoine, R. 288 (1998) 138  
Gong, Q., see Li, J. 288 (1998) 175  
Gonze, X., see Savin, A. 288 (1998) 391  
Gorer, S., see Lifshitz, E. 288 (1998) 188  
Görner, H., Erratum to: "Photochemical ring opening in nitrospiropyrans: triplet pathway and the role of singlet molecular oxygen". [Chem. Phys. Lett. 282 (1998) 381–390] 288 (1998) 589  
Goyal, S., see Scholefield, M.R. 288 (1998) 487  
Gozin, Y., see Uzan, O. 288 (1998) 356  
Gräfenstein, J., E. Kraka and D. Cremer, Density functional theory for open-shell singlet biradicals 288 (1998) 593  
Granlund, T., M. Theander, M. Berggren, M. Andersson, A. Ruzeckas, V. Sundström, G. Björk, M. Granström and O. Inganäs, A polythiophene microcavity laser 288 (1998) 879  
Granström, M., see Granlund, T. 288 (1998) 879  
Graupner, W., see Cerullo, G. 288 (1998) 561

- Grein, F., see Woeller, M. 288 (1998) 603
- Grosse, R., see Isfort, O. 288 (1998) 71
- Gustavsson, T., see Pommeret, S. 288 (1998) 833
- Halas, N.J., see Oldenburg, S.J. 288 (1998) 243
- Hamada, A., see Sueoka, O. 288 (1998) 124
- Hamon, S., J.B.A. Mitchell and B.R. Rowe, Low-temperature measurements of the atomic association reaction  $\text{Ar}^+ + 2\text{Ar} \rightarrow \text{Ar}_2^+ + \text{Ar}$  288 (1998) 523
- Han, K.-L., see Deng, W.-Q. 288 (1998) 33
- Han, K.-L., see Wang, G.-J. 288 (1998) 429
- Han, T.P.J., see Torchia, G.A. 288 (1998) 65
- Hannongbua, S., On the solvation of lithium ions in liquid ammonia: Monte Carlo simulations with a three-body potential 288 (1998) 663
- Hanser, C., see Mordasini, T.Z. 288 (1998) 183
- Hase, W.L., see Bolton, K. 288 (1998) 621
- Hawkins, G.D., see Li, J. 288 (1998) 293
- He, G.-Z., see Deng, W.-Q. 288 (1998) 33
- He, G.-Z., see Wang, G.-J. 288 (1998) 429
- Head, J.D., see Kairys, V. 288 (1998) 423
- Hébert, Ph., see Antoine, R. 288 (1998) 138
- Hedhili, M.N., see Šiller, L. 288 (1998) 776
- Hegstrom, R.A., Spontaneous symmetry breaking in Bose-Einstein condensates 288 (1998) 248
- Hertel, I.V., see Campbell, E.E.B. 288 (1998) 131
- Hidao, S., see Saito, S.L. 288 (1998) 277
- Hitchman, M.A., see Masters, V.M. 288 (1998) 743
- Ho, T.-S., see Hu, X.-G. 288 (1998) 719
- Hobza, P. and J. Šponer, Significant structural deformation of nucleic acid bases in stacked base pairs: an ab initio study beyond Hartree-Fock 288 (1998) 7
- Hobza, P., see Burda, J.V. 288 (1998) 20
- Hodes, G., see Lifshitz, E. 288 (1998) 188
- Horie, O. and G.K. Moortgat, The effect of the addition of CO on the reaction of ozone with ethene 288 (1998) 464
- Hu, X.-G., T.-S. Ho and H. Rabitz, Variational reproducing kernel Hilbert space (RKHS) grid method for quantum mechanical bound-state problems 288 (1998) 719
- Hüttner, W., P. Nowicki and M. Gamperling, Rotational magnetism in the ground and  $(000^01^1)$  vibrational states of trifluorophosphine,  $\text{PF}_3$  288 (1998) 553
- Ikeda, T., see Azuma, J. 288 (1998) 77
- Ikeguchi, M., S. Shimizu, K. Tazaki, S. Nakamura and K. Shimizu, Calculation of temperature dependence of free energy caused by potential function changes 288 (1998) 333
- Inganäs, O., see Granlund, T. 288 (1998) 879
- Isfort, O., B. Boddenberg, F. Fujara and R. Grosse, Molecular dynamics of benzene in zeolite NaY studied by 2D deuteron NMR 288 (1998) 71
- Ishida, T., Y. Fujimura, T. Fujiwara and O. Kajimoto, Excited state dynamics of 9,9'-bi-anthryl clusters with  $\text{H}_2\text{O}$  and Ar 288 (1998) 433
- Ishikawa, M., see Ye, J.Y. 288 (1998) 885
- Iucci, G., see Carravetta, V. 288 (1998) 37
- Iwasawa, Y., see Chun, W.-J. 288 (1998) 868

- Jaques, F., see Torchia, G.A. 288 (1998) 65
- Jellinek, J., S. Srinivas and P. Fantucci, Ab initio Monte Carlo: application to  $\text{Li}_8$  288 (1998) 705
- Jena, P., see Reddy, B.V. 288 (1998) 253
- Jones, T.S., see Mulcahy, C.P.A. 288 (1998) 203
- Jonsson, D., Y. Luo, K. Ruud, P. Norman and H. Ågren, Calculations of circular intensity differences in electric-field-induced second harmonic generation 288 (1998) 371
- Jost, R., see Campargue, A. 288 (1998) 734
- Joubert, D.P., A numerical study of the functional derivative of the kinetic part of the density functional correlation energy 288 (1998) 338
- Kachanov, A., see Campargue, A. 288 (1998) 734
- Kairys, V. and J.D. Head, Electric field effects on the geometry and vibrations of charged molecules: the hydroxide ion case 288 (1998) 423
- Kajimoto, O., see Ishida, T. 288 (1998) 433
- Kassab, E., see Dziekoński, P. 288 (1998) 538
- Khriachtchev, L., M. Pettersson and M. Räsänen, On self-limitation of UV photolysis in rare-gas solids and some of its consequences for matrix studies 288 (1998) 727
- Kim, S.K., see Lim, S.-M. 288 (1998) 828
- Kim, T.-S., see Lim, S.-M. 288 (1998) 828
- Kimura, M., see Sueoka, O. 288 (1998) 124
- Kind, I., T. Berndt and O. Böge, Gas-phase rate constants for the reaction of  $\text{NO}_3$  radicals with a series of cyclic alkenes, 2-ethyl-1-butene and 2,3-dimethyl-1,3-butadiene 288 (1998) 111
- Kitagawa, N., see Kumada, T. 288 (1998) 755
- Kleindienst, P. and G.H. Wagnière, Interferometric detection of magnetochiral birefringence 288 (1998) 89
- Kleinhammes, A., see Bower, C. 288 (1998) 481
- Kobayashi, T., see Matsuse, A. 288 (1998) 165
- Kohama, M., see Sugimoto, T. 288 (1998) 767
- Koto, E., see Furuya, K. 288 (1998) 816
- Kovačević, B. and Z.B. Maksić, Toward engineering of very strong organic bases: pronounced proton affinity of molecules possessing imino structural and electronic motif 288 (1998) 289
- Koyama, Y., see Fujii, R. 288 (1998) 847
- Kraka, E., see Gräfenstein, J. 288 (1998) 593
- Kratzer, P., The dynamics of the  $\text{H} + \text{D}/\text{Si}(001)$  reaction: a trajectory study based on ab initio potentials 288 (1998) 396
- Ku, J.K., see Lee, K. 288 (1998) 531
- Kuki, M., see Fujii, R. 288 (1998) 847
- Kumada, T., N. Kitagawa, T. Noda, J. Kumagai, Y. Aratono and T. Miyazaki, An ENDOR spectrum of H atoms in solid  $\text{H}_2$  288 (1998) 755
- Kumagai, J., see Kumada, T. 288 (1998) 755
- Küppers, J., see Wehner, S. 288 (1998) 873
- Lafargue, P.E., J.J. Gaumet and J.F. Muller, Analysis of thermally treated silica gel using Fourier transform ion cyclotron resonance mass spectrometry 288 (1998) 494
- Laganà, A., A. Riganelli, G. Ochoa de Aspuru, E. Garcia and M.T. Martinez, On multi-quantum vibrational deexcitation in symmetric reactions 288 (1998) 616
- Lamp, J.A. and B. Schramm, Vibrational relaxation of  $\text{HCl}$  ( $\nu = 1$ ) in  $\text{HCl}/\text{CO}_2$  and  $\text{HCl}/\text{CO}_2/\text{argon}$  gaseous mixtures 288 (1998) 83



- Langenaeker, W., F. De Proft, F. Tielens and P. Geerlings, Calculation of adsorption energies of molecules in cages: a density functional approach 288 (1998) 628
- Lanzani, G., see Cerullo, G. 288 (1998) 561
- Lanzani, G., see Wong, K.S. 288 (1998) 59
- Lawruszczuk, R., see Elhanine, M. 288 (1998) 785
- Le Coat, Y., see Šiller, L. 288 (1998) 776
- Lee, K., H.S. Son, S.C. Bae and J.K. Ku, Collisional quenching of Ga(5p) atoms by H<sub>2</sub>, D<sub>2</sub> and CH<sub>4</sub> 288 (1998) 531
- Legon, A.C., see Cooke, S.A. 288 (1998) 441
- Leising, G., see Cerullo, G. 288 (1998) 561
- Li, J., G.D. Hawkins, C.J. Cramer and D.G. Truhlar, Universal reaction field model based on ab initio Hartree-Fock theory 288 (1998) 293
- Li, J., S. Wang, H. Yang, Q. Gong, X. An, H. Chen and D. Qiang, Femtosecond third-order optical nonlinearity of C<sub>60</sub> and its derivative at a wavelength of 810 nm 288 (1998) 175
- Li, M., Z. Xu, X. You, X. Zheng and H. Wang, Photophysical properties of dodecaphenylporphyrins with different substituents 288 (1998) 459
- Li, Y., see Liu, X.-H. 288 (1998) 804
- Lifshitz, E., I. Dag, I. Litvin, G. Hodes, S. Gorer, R. Reisfeld, M. Zelner and H. Minti, Optical properties of CdSe nanoparticle films prepared by chemical deposition and sol-gel methods 288 (1998) 188
- Lim, G.-I., see Lim, S.-M. 288 (1998) 828
- Lim, S.-M., T.-S. Kim, G.-I. Lim, S.K. Kim and Y.S. Choi, Direct formation of CH<sub>2</sub> ( $\tilde{b}^1B_1$ ) in the near-UV photodissociation of diazine 288 (1998) 828
- Lincoln, P., A generalized McGhee-von Hippel method for the cooperative binding of different competing ligands to an infinite one-dimensional lattice 288 (1998) 647
- Linnartz, H., T. Speck and J.P. Maier, High-resolution infrared spectrum of the  $\nu_3$  band in Ar-HCO<sup>+</sup> 288 (1998) 504
- Lipson, M., A.A. Deniz and K.S. Peters, The sub-picosecond dynamics of diphenylmethylchloride ion pairs and radical pairs 288 (1998) 781
- List, E., see Cerullo, G. 288 (1998) 561
- Litvin, I., see Lifshitz, E. 288 (1998) 188
- Liu, X.-H., X.-G. Zhang, Y. Li, X.-Y. Wang and N.-Q. Lou, Cluster formation by direct laser vaporization: evidence for the twofold mechanism 288 (1998) 804
- Loi, M.A., see Bongiovanni, G. 288 (1998) 749
- Lomoth, R. and O. Brede, Spectral and kinetic identification of radical cations of pyrimidine bases by stepwise electron transfer 288 (1998) 47
- López, J.C., see Sanz, M.E. 288 (1998) 760
- Lou, N.-Q., see Liu, X.-H. 288 (1998) 804
- Lou, N.-Q., see Wang, G.-J. 288 (1998) 429
- Ludwigs, H., N. Gador, L.-E. Berg, P. Royen and L. Viktor, Time-resolved optical double resonance spectroscopy of the G<sup>2</sup>Σ<sup>+</sup> state of BaCl 288 (1998) 527
- Luo, Y., see Jonsson, D. 288 (1998) 371
- Luzzati, S., see Bongiovanni, G. 288 (1998) 749
- Ma, B., A.M. Milton and Y.-P. Sun, Infrared spectroscopy of all-carbon poly[60]fullerene polymer and [60]fullerene dimer model 288 (1998) 854
- Ma, N.L., see Siu, F.M. 288 (1998) 408
- Ma, X., see Wang, C. 288 (1998) 473

- Maier, J.P., see Linnartz, H. 288 (1998) 504
- Maksić, Z.B., see Kovačević, B. 288 (1998) 289
- Malmqvist, P.-Å., see Finley, J. 288 (1998) 299
- Malyarevich, A.M., see Yumashev, K.V. 288 (1998) 567
- Mandal, D., see Pal, S.K. 288 (1998) 793
- Manivet, P. and M. Masella, An ab initio study of three (ethane-1,2 diol/water) complexes 288 (1998) 642
- Manthe, U., see Pesce, L. 288 (1998) 383
- Märk, T.D., see Denifl, G. 288 (1998) 105
- Martín, E. and R. Weigand, A correlation between redox potentials and photophysical behaviour of compounds with intramolecular charge transfer: application to N-substituted 1,8-naphthalimide derivatives 288 (1998) 52
- Martin, J.M.L., see Uzan, O. 288 (1998) 356
- Martin, M. and C. Cerezo, Collisional removal of  $CD(A^2\Delta$  and  $B^2\Sigma^-)$  by Xe. Dependence on rotational and vibrational excitation 288 (1998) 799
- Martinez, M.T., see Laganà, A. 288 (1998) 616
- Maruyama, K., see Furuya, K. 288 (1998) 816
- Maruyama, Y., see Ye, J.Y. 288 (1998) 885
- Masella, M., see Manivet, P. 288 (1998) 642
- Masters, V.M., M.J. Riley and M.A. Hitchman, Sharp vibronic spectra of Cu(II) doped  $Cs_2ZrCl_6$  288 (1998) 743
- Matsuse, A., S. Takeuchi, K. Yoshino and T. Kobayashi, Dynamics of photoexcitations in a poly[3-dodecylthiophene] thin film studied by femtosecond visible–near-infrared absorption spectroscopy 288 (1998) 165
- Maynau, D., see Ben-Amor, N. 288 (1998) 348
- Mazyar, O.A. and T. Baer, Theoretical and experimental studies of unimolecular dissociation of phosphorus tribromide ions 288 (1998) 327
- McDowell, C.A., see Ding, S. 288 (1998) 230
- Ménard, M., see Pommeret, S. 288 (1998) 833
- Menzel, A., see Frigo, S.P. 288 (1998) 98
- Mikhailov, V.P., see Yumashev, K.V. 288 (1998) 567
- Milton, A.M., see Ma, B. 288 (1998) 854
- Minti, H., see Lifshitz, E. 288 (1998) 188
- Mishra, M.K., see Vandana, K.S. 288 (1998) 545
- Mitchell, J.B.A., see Hamon, S. 288 (1998) 523
- Mitzner, R., see Campbell, E.E.B. 288 (1998) 131
- Miyazaki, T., see Kumada, T. 288 (1998) 755
- Moiseyev, N., see Zavin, R. 288 (1998) 413
- Moortgat, G.K., see Horie, O. 288 (1998) 464
- Mordasini, T.Z., C. Hanser and W. Thiel, Molecular structure of the fullerene  $C_{70}$  at 825°C: quantum-chemical molecular dynamics simulations 288 (1998) 183
- Moscardó, F., A.J. Pérez-Jiménez, J.C. Sancho-García and E. San Fabián, On the application of the Kohn–Sham theory to the calculation of potential energy curves 288 (1998) 418
- Mühlhäuser, M., see Woeller, M. 288 (1998) 603
- Muigg, D., see Denifl, G. 288 (1998) 105
- Mulcahy, C.P.A., J. Eggeling and T.S. Jones, Low-energy electron beam induced dissociation of methyl groups chemisorbed on semiconductor surfaces:  $(CH_3)_3Al$  adsorbed on GaAs and InSb 288 (1998) 203
- Müllen, K., see Barth, S. 288 (1998) 147



- Muller, J.F., see Lafargue, P.E. 288 (1998) 494
- Munakata, M., see Sugimoto, T. 288 (1998) 767
- Mura, A., see Bongiovanni, G. 288 (1998) 749
- Murphy, R.B. and R.A. Friesner, Accurate quantum chemical calculation of the relative energetics of C<sub>20</sub> carbon clusters via localized multireference perturbation calculations 288 (1998) 403
- Nakajima, N., A selectively enhanced multicanonical molecular dynamics method for conformational sampling of peptides in realistic water molecules 288 (1998) 319
- Nakamura, S., see Ikeguchi, M. 288 (1998) 333
- Nakano, M. and K. Yamaguchi, Numerical coupled Liouville approach: dependence of population differences between excited and ground states on field intensity and size of molecular aggregates 288 (1998) 25
- Naskrecki, R., see Pommeret, S. 288 (1998) 833
- Nishimura, K.-i., see Sugimoto, T. 288 (1998) 767
- Nisoli, M., see Cerullo, G. 288 (1998) 561
- Nobusada, K. and K. Sakimoto, A quantum mechanical study of He + H<sub>2</sub> → He + H + H in the energy range 5–10 eV 288 (1998) 311
- Noda, T., see Kumada, T. 288 (1998) 755
- Norman, P., see Jonsson, D. 288 (1998) 371
- Nowicki, P., see Hüttner, W. 288 (1998) 553
- Nüesch, F., F. Rotzinger, L. Si-Ahmed and L. Zuppiroli, Chemical potential shifts at organic device electrodes induced by grafted monolayers 288 (1998) 861
- Ochoa de Aspuru, G., see Laganà, A. 288 (1998) 616
- Ogawa, T., see Furuya, K. 288 (1998) 816
- Ogino, R., see Takahashi, M. 288 (1998) 714
- Ogino, R., see Takahashi, M. 288 (1998) 821
- Okada, T., see Ye, J.Y. 288 (1998) 885
- Olbrechts, G., see Clays, K. 288 (1998) 171
- Oldenburg, S.J., R.D. Averitt, S.L. Westcott and N.J. Halas, Nanoengineering of optical resonances 288 (1998) 243
- Olsen, J. and D. Sundholm, On perturbation expansions of the extended Koopmans' theorem 288 (1998) 282
- Onaka, K., see Fujii, R. 288 (1998) 847
- Pal, S.K., A. Datta, D. Mandal and K. Bhattacharyya, Photoisomerisation of diethyloxadi-carbocyanine iodide in micelles 288 (1998) 793
- Paolucci, G., see Carravetta, V. 288 (1998) 37
- Papadopoulos, M.G. and A.J. Sadlej, Interaction effects on electric susceptibilities: A model study of polarizabilities of the Be atom embedded in He clusters 288 (1998) 377
- Parrinello, M., see Trout, B.L. 288 (1998) 343
- Pérez-Jiménez, A.J., see Moscardó, F. 288 (1998) 418
- Persoons, A., see Clays, K. 288 (1998) 171
- Pesce, L., T. Gerds, U. Manthe and P. Saalfrank, Variational wave packet method for dissipative photodesorption problems 288 (1998) 383
- Peters, K.S., see Lipson, M. 288 (1998) 781
- Pettersson, M., see Khriachtchev, L. 288 (1998) 727
- Peyerimhoff, S.D., see Woeller, M. 288 (1998) 603

- Piaggi, A., see Bongiovanni, G. 288 (1998) 749
- Pines, E., A new derivation of approximate limiting laws for ionic activities 288 (1998) 270
- Poluektov, O.G. and A.A. Doubinski, Two-dimensional high-field electron spin echo spectroscopy of nitroxide spin probes 288 (1998) 841
- Polzonetti, G., see Carravetta, V. 288 (1998) 37
- Pommeret, S., R. Naskrecki, P. van der Meulen, M. Ménard, G. Vigneron and T. Gustavsson, Ultrafast events in the electron photodetachment from the hexacyanoferrate(II) complex in solution 288 (1998) 833
- Posnov, N.N., see Yumashev, K.V. 288 (1998) 567
- Pushpalatha, K. and M.V. Sangaranarayanan, Phase transitions at electrochemical interfaces: Evaluation of critical exponents for condensation of organic adsorbates 288 (1998) 216
- Pyykkö, P., see Burda, J.V. 288 (1998) 635
- Qiang, D., see Li, J. 288 (1998) 175
- Rabitz, H., see Hu, X.-G. 288 (1998) 719
- Radloff, W., see Farmanara, P. 288 (1998) 518
- Räsänen, M., see Khriachtchev, L. 288 (1998) 727
- Rausch, H., see Braun, T. 288 (1998) 179
- Reddy, B.V. and P. Jena, Signature of crystalline order in ultra-small metal-oxide clusters 288 (1998) 253
- Reisfeld, R., see Lifshitz, E. 288 (1998) 188
- Reisler, H., see Scholefield, M.R. 288 (1998) 487
- Riganelli, A., see Laganà, A. 288 (1998) 616
- Riley, M.J., see Masters, V.M. 288 (1998) 743
- Rizzo, A., see Fernández, B. 288 (1998) 677
- Rollins, H.W., see Sun, Y.-P. 288 (1998) 585
- Roos, B.O., see Finley, J. 288 (1998) 299
- Rossi, E., see Ben-Amor, N. 288 (1998) 348
- Rotzinger, F., see Nüesch, F. 288 (1998) 861
- Rowe, B.R., see Hamon, S. 288 (1998) 523
- Royen, P., see Ludwigs, H. 288 (1998) 527
- Runeberg, N., see Burda, J.V. 288 (1998) 635
- Russo, M.V., see Carravetta, V. 288 (1998) 37
- Ruud, K., see Jonsson, D. 288 (1998) 371
- Ruzeckas, A., see Granlund, T. 288 (1998) 879
- Saalfrank, P., see Pesce, L. 288 (1998) 383
- Sadlej, A.J., see Papadopoulos, M.G. 288 (1998) 377
- Safont, V.S., J. Andrés and L.R. Domingo, A theoretical study on the decomposition mechanism of  $\beta$ -propiolactone and  $\beta$ -butyrolactone 288 (1998) 261
- Saito, S.L. and S. Hidao, Theoretical study on the stability of PsBr and PsI with second-order correlation energies 288 (1998) 277
- Sakimoto, K., see Nobusada, K. 288 (1998) 311
- Sancho-García, J.C., see Moscardó, F. 288 (1998) 418
- San Fabián, E., see Moscardó, F. 288 (1998) 418
- Sangaranarayanan, M.V., see Pushpalatha, K. 288 (1998) 216
- Sanz-García, J.A., see Torchia, G.A. 288 (1998) 65
- Sanz, M.E., J.C. López and J.L. Alonso, Rotational spectrum and structure of the tetrahydrothiophene  $\cdots$  hydrogen fluoride complex 288 (1998) 760

- Sathyamurthy, N., see Vandana, K.S. 288 (1998) 545
- Sato, H., see Sueoka, O. 288 (1998) 124
- Savin, A., C.J. Umrigar and X. Gonze, Relationship of Kohn-Sham eigenvalues to excitation energies 288 (1998) 391
- Scherf, U., see Barth, S. 288 (1998) 147
- Schlegel, H.B., see Bolton, K. 288 (1998) 621
- Scholefield, M.R., J.-H. Choi, S. Goyal and H. Reisler, Endoergic reactions of hyperthermal C(<sup>3</sup>P) with methane and acetylene 288 (1998) 487
- Schramm, B., see Lamp, J.A. 288 (1998) 83
- Schwartz, B.J., see Doan, V. 288 (1998) 576
- Selçuki, C. and V. Aviyente, A DFT study of carbonyl oxide and its methyl-substituted analogues in solution 288 (1998) 669
- Sergeyev, N.M., see Torocheshnikov, V.N. 288 (1998) 809
- Serrano-Andrés, L., see Finley, J. 288 (1998) 299
- Shaik, S., see Filatov, M. 288 (1998) 689
- Shimizu, K., see Ikeguchi, M. 288 (1998) 333
- Shimizu, S., see Ikeguchi, M. 288 (1998) 333
- Shishido, A., see Azuma, J. 288 (1998) 77
- Shiwaku, K., see Sugimoto, T. 288 (1998) 767
- Si-Ahmed, L., see Nüesch, F. 288 (1998) 861
- Šiller, L., M.N. Hedhili, Y. Le Coat, M. Tronc and R. Azria, Synthesis of dioxygen in a CO<sub>2</sub> matrix: Positive ion desorption at the solid ionisation threshold 288 (1998) 776
- Siu, F.M., N.L. Ma and C.W. Tsang, Theoretical binding energies of lithium ions to short-chain alcohols 288 (1998) 408
- Skinner, J.L., see Geva, E. 288 (1998) 225
- Smets, J., see Smith, D.M.A. 288 (1998) 609
- Smith, D.M.A., J. Smets, Y. Elkadi and L. Adamowicz, Ab initio theoretical study of dipole-bound anions of molecular complexes. [H<sub>2</sub>O ··· HCN]<sup>-</sup> and [HCN ··· H<sub>2</sub>O]<sup>-</sup> anions 288 (1998) 609
- Soep, B., see Elhanine, M. 288 (1998) 785
- Sokalski, W.A., see Dziekoński, P. 288 (1998) 538
- Son, H.S., see Lee, K. 288 (1998) 531
- Song, K., see Bolton, K. 288 (1998) 621
- Speck, T., see Linnartz, H. 288 (1998) 504
- Šponer, J., see Hobza, P. 288 (1998) 7
- Srinivas, S., see Jellinek, J. 288 (1998) 705
- Stagira, S., see Cerullo, G. 288 (1998) 561
- Stamatovic, A., see Denifl, G. 288 (1998) 105
- Stert, V., see Farmanara, P. 288 (1998) 518
- Suenaga, Y., see Sugimoto, T. 288 (1998) 767
- Sueoka, O., H. Takaki, A. Hamada, H. Sato and M. Kimura, Total cross-sections of electron and positron collisions with CHF<sub>3</sub> molecules: a comparative study with CH<sub>4</sub> and CF<sub>4</sub> 288 (1998) 124
- Sugimoto, T., K. Ueda, S. Endo, N. Toyota, T. Tada, K.-i. Nishimura, M. Kohama, K. Shiwaku, K. Yamamoto, T. Yamaguchi, Y. Suenaga and M. Munakata, 1:2 Dimethyl-substituted tetracyanoquinodimethane. Its radical anion mixed salts: ferromagnetic behavior and high electrical conductivity at room temperature 288 (1998) 767



- Sun, Y.-P. and H.W. Rollins, Preparation of polymer-protected semiconductor nanoparticles through the rapid expansion of supercritical fluid solution 288 (1998) 585  
Sun, Y.-P., see Ma, B. 288 (1998) 854  
Sundholm, D., see Olsen, J. 288 (1998) 282  
Sundström, V., see Granlund, T. 288 (1998) 879  
Sviridov, D.V., see Yumashev, K.V. 288 (1998) 567  
Szlaferek, A., see Danielewicz-Ferchmin, I. 288 (1998) 197
- Tada, T., see Sugimoto, T. 288 (1998) 767  
Takahashi, M., R. Ogino and Y. Udagawa, An electron momentum spectroscopy study of  $\pi$  orbitals of norbornadiene and 1,4-cyclohexadiene: evidence for through-space and through-bond interactions 288 (1998) 714  
Takahashi, M., R. Ogino and Y. Udagawa, Outer valence electronic structure of pyrrole studied by electron momentum spectroscopy 288 (1998) 821  
Takaki, H., see Sueoka, O. 288 (1998) 124  
Takeuchi, S., see Matsuse, A. 288 (1998) 165  
Talbi, D. and Y. Ellinger, Potential energy surfaces for the electronic dissociative recombination of  $\text{HCNH}^+$ : astrophysical implications on the HCN/HNC abundance ratio 288 (1998) 155  
Tamai, N., see Azuma, J. 288 (1998) 77  
Tamburello-Luca, A.A., see Antoine, R. 288 (1998) 138  
Tazaki, K., see Ikeguchi, M. 288 (1998) 333  
Theander, M., see Granlund, T. 288 (1998) 879  
Thiel, W., see Mordasini, T.Z. 288 (1998) 183  
Tian, C. and C.R. Vidal, Cross sections of electron impact ionization of ethylene 288 (1998) 499  
Tielens, F., see Langenaeker, W. 288 (1998) 628  
Torchia, G.A., J.A. Sanz-García, J. Díaz-Caro, F. Jaque and T.P.J. Han, Redistribution of  $\text{Cr}^{3+}$  ions from  $\text{Li}^+$  to  $\text{Nb}^{5+}$  sites in  $\text{ZnO}$  codoped  $\text{LiNbO}_3$ :Cr crystals 288 (1998) 65  
Torochevnikov, V.N. and N.M. Sergeyev,  $^{35}\text{Cl}$  and  $^{37}\text{Cl}$  nuclear magnetic resonance of chloroorganic compounds 288 (1998) 809  
Toyota, N., see Sugimoto, T. 288 (1998) 767  
Tran, V., see Doan, V. 288 (1998) 576  
Tronc, M., see Šiller, L. 288 (1998) 776  
Trout, B.L. and M. Parrinello, The dissociation mechanism of  $\text{H}_2\text{O}$  in water studied by first-principles molecular dynamics 288 (1998) 343  
Truhlar, D.G., see Li, J. 288 (1998) 293  
Tsang, C.W., see Siu, F.M. 288 (1998) 408
- Udagawa, Y., see Takahashi, M. 288 (1998) 714  
Udagawa, Y., see Takahashi, M. 288 (1998) 821  
Ueda, K., see Sugimoto, T. 288 (1998) 767  
Ueda, T., see Furuya, K. 288 (1998) 816  
Umrigar, C.J., see Savin, A. 288 (1998) 391  
Uzan, O., Y. Gozin and J.M.L. Martin, Modeling stabilization of  $\text{Si}=\text{O}$  bonds by Pd/Pt complexes using density functional theory 288 (1998) 356
- Vandana, K.S., N. Chakrabarti, N. Sathyamurthy and M.K. Mishra, Validation of photodissociation models using Raman excitation Profiles: an application to IBr 288 (1998) 545  
Van der Meulen, P., see Pommeret, S. 288 (1998) 833

- Veyret, V., see Campargue, A. 288 (1998) 734
- Vidal, C.R., see Tian, C. 288 (1998) 499
- Vigneron, G., see Pommeret, S. 288 (1998) 833
- Vikor, L., see Ludwigs, H. 288 (1998) 527
- Vorobeichik, I., see Zavin, R. 288 (1998) 413
- Wagnière, G.H., see Kleindienst, P. 288 (1998) 89
- Wang, C., C. Chen, J. Dai and X. Ma, Laser-induced fluorescence studies of jet-cooled  $\text{CF}_2$ : determination of  $\tilde{\text{A}}$ -state stretching frequencies 288 (1998) 473
- Wang, G.-J., R.-S. Zhu, H. Zhang, K.-L. Han, G.-Z. He and N.-Q. Lou, Photodissociation of chlorobenzene at 266 nm 288 (1998) 429
- Wang, H., see Li, M. 288 (1998) 459
- Wang, H., see Wong, K.S. 288 (1998) 59
- Wang, S., see Li, J. 288 (1998) 175
- Wang, X.-Y., see Liu, X.-H. 288 (1998) 804
- Watanabe, Y., see Fujii, R. 288 (1998) 847
- Wehner, S. and J. Küppers, Two consecutive Eley-Rideal reaction steps in a D atom/adsorbate interaction: from methylene iodide via methyl iodide to methane 288 (1998) 873
- Weigand, R., see Martín, E. 288 (1998) 52
- Westcott, S.L., see Oldenburg, S.J. 288 (1998) 243
- Wimperis, S., see Ashbrook, S.E. 288 (1998) 509
- Woeller, M., M. Mühlhäuser, S.D. Peyerimhoff and F. Grein, Chemisorption of ethylene on  $\text{Si}_5^+$  cluster ions. A theoretical study 288 (1998) 603
- Wong, K.S., H. Wang and G. Lanzani, Ultrafast excited-state planarization of the hexamethylsexithiophene oligomer studied by femtosecond time-resolved photoluminescence 288 (1998) 59
- Wu, Y., see Bower, C. 288 (1998) 481
- Xu, Z., see Li, M. 288 (1998) 459
- Yamaguchi, K., see Nakano, M. 288 (1998) 25
- Yamaguchi, T., see Sugimoto, T. 288 (1998) 767
- Yamamoto, K., see Sugimoto, T. 288 (1998) 767
- Yang, H., see Li, J. 288 (1998) 175
- Ye, J.Y., M. Ishikawa, O. Yogi, T. Okada and Y. Maruyama, Bimodal site distribution of a polymer film revealed by flexible single-molecule probes 288 (1998) 885
- Yogi, O., see Ye, J.Y. 288 (1998) 885
- Yoshino, K., see Matsuse, A. 288 (1998) 165
- You, X., see Li, M. 288 (1998) 459
- Yumashev, K.V., A.M. Malyarevich, N.N. Posnov, I.A. Denisov, V.P. Mikhailov, M.V. Artemyev and D.V. Sviridov, Optical transient bleaching of photochromic polytungstic acid 288 (1998) 567
- Zahradník, R., see Burda, J.V. 288 (1998) 20
- Zavin, R., I. Vorobeichik and N. Moiseyev, Motion of wave-packets using the smooth-exterior-scaling complex potential 288 (1998) 413
- Zelner, M., see Lifshitz, E. 288 (1998) 188
- Zerbetto, F., see Campbell, E.E.B. 288 (1998) 131
- Zhan, C.-G. and C.-J. Zhang, Ab initio configuration interaction studies on the photoelectron spectra of chlorine nitrate 288 (1998) 15

Zhan, J.-P., see Deng, W.-Q.	288 (1998) 33
Zhang, C.-J., see Zhan, C.-G.	288 (1998) 15
Zhang, H., see Wang, G.-J.	288 (1998) 429
Zhang, X.-G., see Liu, X.-H.	288 (1998) 804
Zheng, X., see Li, M.	288 (1998) 459
Zhou, O., see Bower, C.	288 (1998) 481
Zhu, R.-S., see Wang, G.-J.	288 (1998) 429
Zuppiroli, L., see Nüesch, F.	288 (1998) 861